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A METHOD FOR THE CALCULATION OF LARGE NUMBERS OF DIPOLE AND QUADRUPOLE TRANSITION PROBABILITIES

*by Lawrence P. Shomo, Goetz K. Oertel,
and Charles S. Freer*

*Langley Research Center
Hampton, Va. 23365*



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1. Report No. NASA TN D-5987		2. Government Accession No.		3. Recipient's Catalog No.	
4. Title and Subtitle A METHOD FOR THE CALCULATION OF LARGE NUMBERS OF DIPOLE AND QUADRUPOLE TRANSITION PROBABILITIES				5. Report Date November 1970	
7. Author(s) Lawrence P. Shomo, Goetz K. Oertel (NASA Headquarters), and Charles S. Freer (Clarkson College of Technology)				6. Performing Organization Code	
9. Performing Organization Name and Address NASA Langley Research Center Hampton, Va. 23365				8. Performing Organization Report No. L-7109	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D.C. 20546				10. Work Unit No. 129-02-22-02	
15. Supplementary Notes				11. Contract or Grant No.	
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17. Key Words (Suggested by Author(s)) Atomic spectroscopy Coulomb approximation Dipole and quadrupole transition probabilities Computer program				14. Sponsoring Agency Code	
19. Security Classif. (of this report) Unclassified		20. Security Classif. (of this page) Unclassified		21. No. of Pages 39	
				22. Price* \$3.00	
18. Distribution Statement Unclassified - Unlimited					

A METHOD FOR THE CALCULATION OF LARGE NUMBERS OF DIPOLE AND QUADRUPOLE TRANSITION PROBABILITIES

By Lawrence P. Shomo, Goetz K. Oertel,^{*}
and Charles S. Freer[†]
Langley Research Center

SUMMARY

A computer program is presented which selects allowed transitions and calculates dipole and quadrupole transition probabilities for transitions with LS coupling and no equivalent electrons, based on an extension of the Coulomb approximation formalism to quadrupole and higher multipole transitions. Absorption oscillator strengths or f-values calculated by (1) the self-consistent-field method, (2) the scaled Thomas-Fermi method, (3) the Coulomb approximation method, (4) the variational method, and (5) the effective charge method for singlet and triplet transitions in neutral helium are presented and compared. The Coulomb approximation f-values calculated with the present computer program are found to be in good agreement with the results obtained by the more sophisticated methods.

INTRODUCTION

The present status of the knowledge of transition probabilities or of absorption oscillator strengths (f-values) is poor compared with that of the wavelengths of atomic spectral lines. The f-values are known only for a small number of the lines for which wavelengths are known, and the accuracy of the available values is usually poor.

The calculation of f-values requires a knowledge of the wave functions of the two states involved in the transition. It is necessary to employ approximations to determine the wave functions for nonhydrogenic atoms or ions since Schrödinger's equation can be solved analytically only for the simple one-electron atom case. Several techniques that provide approximate wave functions have been developed. The most sophisticated technique of these is the self-consistent-field method (refs. 1, 2, and 3). Provided that exchange and correlation effects are considered, f-values can be obtained which should not deviate from the true values by more than 20 percent. Solution by numerical

^{*}NASA Headquarters, Washington, D.C.

[†]Clarkson College of Technology, Potsdam, New York.

techniques on a computer is almost mandatory because of the complexity and iterative nature of the self-consistent-field calculations. The computing time still becomes excessive when very complicated systems (many-electron systems) are considered.

The scaled Thomas-Fermi method (ref. 4) provides a useful alternative. This method is not subject to some of the limitations of the Coulomb approximation method and is thus more generally applicable. Its accuracy is, of course, limited by the validity of the Thomas-Fermi model of the atom's or ion's core (inner electrons plus nucleus). The adjustment of a scaling factor, however, to provide energy values consistent with the measured values allows for some compensation for the model's inadequacies. Even for relatively simple systems, the computation time for the scaled Thomas-Fermi method is less than that for the self-consistent-field method by at least one order of magnitude.

The Coulomb approximation method (ref. 5) is applicable to many lines of interest, and for those transitions where its assumptions are met, it gives f -values which are in close agreement with the self-consistent-field results. Even for relatively simple systems where the time required for self-consistent-field calculations is still relatively short, the Coulomb approximation method will result in a reduction of computing time by about three orders of magnitude.

Radial matrix elements for the Coulomb approximation method can be fully characterized by the effective principal quantum numbers and the individual electron orbital angular momentum quantum numbers of the two levels involved in the transition. Thus, generalized tables can be assembled in terms of these quantum numbers alone. In this sense the Coulomb approximation method has a distinct advantage over the other two methods.

The Coulomb approximation method is attractive because of its simplicity and wide range of applicability. Oertel and Shomo (ref. 6) extended the Coulomb approximation formalism to the multipole case and presented extensive tables for computing Coulomb approximation radial matrix elements for dipole transitions s-p, p-d, d-f, f-g, g-h, and h-i, and for quadrupole transitions p-p, d-d, f-f, g-g, h-h, i-i, s-d, p-f, d-g, f-h, g-i, and h-j. The extension of the Coulomb approximation method to higher multipole transitions was deemed desirable because of the need for knowledge of forbidden electric-multipole transition probabilities in astrophysics and because large numbers of matrix elements, both dipole and quadrupole, are required for computations of the Stark broadening of isolated ion lines (ref. 7).

The purpose of this paper is to present a FORTRAN IV computer program which selects allowed transitions and calculates Coulomb approximation line strengths and transition probabilities for dipole and quadrupole transitions with LS coupling and no equivalent electrons, based upon the formulae presented in reference 6, and to compare the

Coulomb approximation f-values with results obtained from more sophisticated calculations for neutral helium. A listing of the computer program is presented in appendix A.

SYMBOLS

$A(\alpha, \alpha')$	dipole or quadrupole transition probability, second ⁻¹
$a_k, a_{k'}$	coefficients generated from recurrence relation (eq. (8))
a_0	Bohr radius, centimeters
c	velocity of light in vacuum, centimeters/second
$E_{n^*, l}$	measured binding energy of orbit with quantum numbers n^* and l , centimeter ⁻¹
e	elementary charge
$f(\alpha, \alpha')$	absorption oscillator strength, dimensionless
$g_\alpha, g_{\alpha'}$	statistical weight of level α and level α' , respectively, dimensionless
\hbar	Planck's constant/ 2π , erg-seconds
I	radial factor, $(-1)^{l' - l} \sqrt{l'}$ I_S
I_S	radial transition integral
J	total atomic angular momentum quantum number, dimensionless
k, k'	summation indices, dimensionless
L	total atomic orbital angular momentum quantum number, dimensionless
ΔL	change in total atomic orbital angular momentum quantum number for a transition
L_1	total atomic orbital angular momentum quantum number of parent configuration, dimensionless

l, l'	individual electron orbital angular momentum quantum numbers, dimensionless
$l_>$	larger of the individual electron orbital angular momentum quantum numbers of two states involved in transition, dimensionless
$l_<$	smaller of the individual electron orbital angular momentum quantum numbers of two states involved in transition, dimensionless
n, n'	effective (noninteger) principal quantum numbers, dimensionless
n^*	integer principal quantum number, dimensionless
Δn^*	absolute magnitude of change of principal quantum number in a transition, dimensionless
$R(n, l), R(n', l')$	normalized radial wave functions, atomic units
R_{line}	line factor, dimensionless
R_{mult}	multiplet factor, dimensionless
R_∞	Rydberg constant, centimeter ⁻¹
r	magnitude of position vector, atomic units (a_0)
S	total atomic spin quantum number, dimensionless
$S(\text{line})$	relative line strength, dimensionless
$S(\text{mult})$	relative multiplet strength, dimensionless
$S(\alpha, \alpha')$	line strength, atomic units $\left(a_0^2 e^2 \text{ for } s = 1, a_0^4 e^2 \text{ for } s = 2 \right)$
s	index (1 for dipole, 2 for quadrupole)
$T_\alpha, T_{\alpha'}$	term value of level α and level α' , respectively, centimeter ⁻¹
T_∞	term value of series limit, centimeter ⁻¹

$W(abcd;ef)$	Racah coefficient, dimensionless
Z	charge of nucleus minus charge of inner electrons, dimensionless
Z^*	effective charge, dimensionless
α	lower level
α'	excited level
Γ	gamma function
λ	transition wavelength, angstroms
σ	dipole radial factor

DEFINITIONS

The dipole absorption oscillator strength or f-value $f(\alpha, \alpha')$ and the transition probability $A(\alpha, \alpha')$ for a transition between an excited level α' and a lower level α can be expressed in terms of the dipole line strength $S(\alpha, \alpha')$ by

$$f(\alpha, \alpha') = \frac{1}{3} \frac{1}{g_{\alpha}} \frac{|T_{\alpha} - T_{\alpha'}|}{R_{\infty}} \frac{S(\alpha, \alpha')}{e^2 a_0^2} \quad (1)$$

and

$$A(\alpha, \alpha') = \frac{1}{6} \left(\frac{e^2}{\hbar c} \right)^4 \frac{c}{a_0} \frac{1}{g_{\alpha'}} \left(\frac{|T_{\alpha} - T_{\alpha'}|}{R_{\infty}} \right)^3 \frac{S(\alpha, \alpha')}{e^2 a_0^2} \quad (2)$$

where a_0 is the Bohr radius, T_{α} , $T_{\alpha'}$, g_{α} , and $g_{\alpha'}$ are the term values and statistical weights of the levels α and α' , respectively, R_{∞} is the Rydberg constant, and c , e , and \hbar have their usual meanings.

The line strength can be factored into angular and radial factors, that is,

$$S(\alpha, \alpha') = S(\alpha', \alpha) = S(\text{line})S(\text{mult})\sigma^2 \quad (3)$$

where the angular part is composed of the relative line strength $S(\text{line})$ and the relative multiplet strength $S(\text{mult})$. The dipole radial factor σ^2 is related to the radial

transition integral I_s ($s = 1$ for the dipole case) by

$$\sigma^2 = \frac{I_{s=1}^2}{4l_{>}^2 - 1} \quad (4)$$

where

$$I_s = \int_0^\infty R(n,l)R(n',l')r^s dr \quad (5)$$

$l_{>}$ is the larger of the individual electron orbital angular momentum quantum numbers l and l' , and $R(n,l)$ and $R(n',l')$ are the normalized radial wave functions of the active electron in atomic units. Relations for the angular factors of the dipole line strength are given in appendix B.

Analogous expressions for the transition probability and line strength for quadrupole transitions are given in appendix C, and they are discussed in detail in reference 6.

COULOMB APPROXIMATION

Bates and Damgaard (ref. 5) assert that for most transitions the potential approximates closely its asymptotic ($r \rightarrow \infty$) Coulomb form in the region of dominant contribution to the transition integral I_s . This is due to the emphasis placed on long radial distances by the factor r^s in I_s , an emphasis which becomes greater with an increase in s , that is, higher multipole transitions. At sufficiently large electron-nucleus separations, the active electron is outside the core of inner electrons and is acted upon by a potential which is very nearly Coulombic. The Coulomb approximation wave functions are obtained by solving the standard central-field radial Schrödinger equation using the Coulomb potential, subject to the condition that the solutions approach zero at large r . The additional constraint that the energy parameter in the Schrödinger equation be identified with the experimentally determined binding energy of the level is imposed. Since the energy parameter defined in this manner is not, in general, an eigenvalue of the Schrödinger equation, the solutions diverge at the origin.

In terms of the Coulomb approximation wave functions R , the radial transition integral I_s ($s = 1$ for dipole, $s = 2$ for quadrupole, etc.) for transitions between levels (n,l) and (n',l') is obtained from

$$I_s = \int_0^\infty R(n,l)R(n',l')r^s dr$$

$$= \frac{2^{n+n'} Z^{n+n'+1}}{n^{n+1} (n')^{n'+1}} \left[\Gamma(n+l+1) \Gamma(n-l) \Gamma(n'+l'+1) \Gamma(n'-l') \right]^{-1/2} \sum_{k=0}^\infty \sum_{k'=0}^\infty a_k a_{k'} \left[\int_0^\infty e^{-rZ(n+n'/nn')} r^{n+n'+s-k-k'} dr \right] \quad (6)$$

where Γ denotes the gamma function. The principal quantum numbers n and n' are noninteger (except for hydrogenic configurations) "effective" principal quantum numbers and may be obtained from

$$n = Z \left(\frac{109737}{T_{\infty} - T} \right)^{1/2} \quad (7)$$

in terms of the series limit T_{∞} (in units cm^{-1}), the measured term value T , and Z the charge of the nucleus minus that of the inner (core) electrons (i.e., $Z = 1$ for neutral atoms). The normalization factor proposed by Hartree (ref. 8) for hydrogenic radial wave functions was used although it is not accurate for noninteger principal quantum numbers. The error thus introduced, however, was shown to be quite small for most cases of interest (ref. 6). The coefficients a_k were generated from the recurrence relation

$$a_k = \frac{n a_{k-1}}{2kZ} \left[l(l+1) - (n-k)(n-k+1) \right] \quad (8)$$

with $a_0 = 1$. The coefficients $a_{k'}$ are given by equation (8) with n and l replaced by n' and l' , respectively, and with $a_{0'} = 1$. The integral over the exponential function in equation (6) can be evaluated as

$$\left[\frac{n n'}{Z(n+n')} \right]^{n+n'+s+1-k-k'} \Gamma(n+n'+s+1-k-k') \quad (9)$$

In order to avoid the divergence of the wave functions at the origin, the summation is cut off by the condition $k+k' < n+n'+s-2$, which amounts to neglecting powers of r less than 2 in equation (6). Thus, the basic assumptions of the Coulomb approximation of Bates and Damgaard are violated when the contribution to the transition integral is large in the core and small at long distances (i.e., when the active electron is in an inner orbital with very small amplitude outside the core, or due to cancellation outside the core region).

COMPUTER PROGRAM

A FORTRAN IV computer program was written to calculate dipole f -values, and both dipole and quadrupole wavelengths, transition probabilities, and line strengths for all of the allowed (dipole and quadrupole) transitions for a given element and stage of ionization. The program is restricted to levels with LS coupling and no equivalent electrons. It calculates the radial matrix elements by the Coulomb approximation formalism developed in reference 6 and described in the present paper. The program is based upon the equations presented in this paper and is listed in appendix A.

The transition parameters can be calculated for all the allowed transitions in a given element and stage of ionization, or the transition parameters can be calculated only for certain allowed transitions by restricting the input data to only those levels involved in the desired transitions. The program operates as follows. The program selects one of the input levels as the initial level and then scans all other levels and applies dipole and quadrupole selection rules to determine the allowed final levels. As each final level is determined, the required transition parameters are calculated. Then, another level is selected as the initial level and the process is repeated. This procedure continues until all the input levels have been chosen as the initial level.

The Coulomb approximation method described in this paper and in reference 6 is utilized in subroutine BATES. The output of this subroutine (RSQUAR) is the value of the radial transition integral squared, that is, I_S^2 . Racah coefficients (ref. 9) are calculated in subroutine RACAH according to the relation

$$W(abcd;ef) = (-1)^{a+b+c+d} \Delta(abe)\Delta(bdf)\Delta(afc)\Delta(edc) \times \sum_{\beta} (-1)^{\beta} (\beta + 1)! [\beta - a - b - e]! \\ \times (\beta - b - d - f)! (\beta - a - f - c)! (\beta - e - d - c)! (a + b + c + d - \beta)! \\ \times (a + d + e + f - \beta)! (b + c + e + f - \beta)! \quad (10)$$

where

$$\Delta(ijk) = \left[\frac{(i + j - k)! (j + k - i)! (k + i - j)!}{(i + j + k + 1)!} \right]^{1/2} \quad (11)$$

is calculated in subroutine DELTA and where the summation in equation (10) is over those integer values of β for which the factorials are meaningful. Extensive tables of Racah coefficients are available (ref. 10).

The computer program offers several options controlled by a set of option variables as follows. When OPQUA = 1, only dipole transitions will be calculated; but when OPQUA = 2, both dipole and quadrupole transitions will be calculated. When OPFVA = 1, dipole f-values and dipole transition probabilities will be calculated; when OPFVA = 2, no f-values or transition probabilities will be calculated; and when OPFVA = 3, dipole f-values and dipole plus quadrupole transition probabilities will be calculated. The line strength, wavelength, and the angular frequency are calculated regardless of the value of OPFVA. The option controlled by NPROP was introduced to provide an easy means of checking the program results by hand calculation. This option provides the entry values for the tables of Coulomb approximation radial matrix elements that were presented in reference 6. The correct value of the radial matrix element for use in the hand calculation can thus be obtained from these tables. When NPROP = 1, these table-entry values

will be printed out for each transition; but when $NPROP = 2$, they will not. The value of the option variable $NLITO$ is the upper limit of Δn^* (the absolute magnitude of the difference between the integer principal quantum numbers for the two levels involved in the transition). The program will not consider any transitions with Δn^* greater than $NLITO$. An upper limit is set on $NLITO$ by statements in the program which require $NLITO \leq 9.0$. The first input card contains the values of these four option variables $OPQUA$, $OPFVA$, $NPROP$, $NLITO$ as required by **FORMAT** statement 140.

The second and third input cards contain information defining the atomic system under consideration. The second card contains the following input variables:

ELEMNO	atomic number of element
Z	core charge of atomic system
NOLEV	number of input terms (NOLEV is independent of J-values) Any number ≤ 90 of no-equivalent electron and LS coupling terms can be used.
NOSER	number of series in atomic system (the limit $NOSER < 10$ is contained in the program)

The second input card contains the values of the variables **ELEMNO**, **Z**, **NOLEV**, and **NOSER** as required by **FORMAT** statement 3.

There will be **NOSER** input cards like the third card, that is, one card is required for each series. Each card will contain the following input variables:

CAPSS(I)	total atomic spin quantum number of Ith series designation
CAPLS(I)	total atomic orbital angular momentum quantum number of Ith series designation
SLIM(I)	series limit (in units cm^{-1}) of Ith series

Thus, the next **NOSER** input cards (starting with the third input card) each contain the values of the variables **CAPSS(I)**, **CAPLS(I)**, and **SLIM(I)** for one of the **NOSER** series as required by **FORMAT** statement 7.

The next series of input cards define the terms of the atomic system. A sequence of two input cards is required for each term. There are **NOLEV** of these two-card

sequences for the atomic system. The first card of the sequence contains the following input variables:

NLITT(I)	principal quantum number of Ith term
LLITT(I)	individual electron orbital angular momentum quantum number of Ith term
CAPS(I)	total atomic spin quantum number of Ith term designation
CAPL(I)	total atomic orbital angular momentum quantum number of Ith term designation
PARITY(I)	parity of Ith term (PARITY(I) = 0,2 means odd or even parity, respectively)
CAPSP(I)	total atomic spin quantum number of Ith term's parent configuration
CAPLP(I)	total atomic orbital angular momentum quantum number of Ith term's parent configuration

Thus, the first card of each two-card sequence defining a term contains the values of the variables NLITT(I), LLITT(I), CAPS(I), CAPL(I), PARITY(I), CAPSP(I), and CAPLP(I) as required by FORMAT statement 6.

There are NOJ J-values (total atomic angular momentum quantum numbers) corresponding to a given term, where NOJ is an integer ≥ 1 calculated in the program. The second card in the two-card sequence contains the energy level values of the term corresponding to each of the term's J-values (i.e., TJ(N,I), N = 1,NOJ (of the Ith term)). The term values must be listed on the card in order of increasing J-value. TJ(N,I) is the energy level (in units cm^{-1}) of the Ith term and Nth J-value. Thus, the second card of each two-card sequence defining a term contains the values of the variables TJ(1,I), TJ(2,I), . . . , TJ(NOJ,I) as required by FORMAT statement 4.

In order to clarify the foregoing instructions, a sample input deck is listed at the end of the program in appendix A. This sample input deck contains six levels of neutral helium, namely, $2s(2S)^3S_1$, $2p(2S)^3P_{0,1,2}^0$, $3p(2S)^3P_{0,1,2}^0$, $3d(2S)^3D_{1,2,3}$, $4p(2S)^3P_{0,1,2}^0$, $4d(2S)^3D_{1,2,3}$ (where the superscript 0 indicates odd parity). The term values used are those of C. E. Moore (ref. 11). Comment cards have been inserted in the sample input deck to explain each input data card.

A sample computer program printout follows the sample input deck listing in appendix A. This printout is a partial printout for the sample input deck (partial in that only the printout is given for the case in which the $2s(2S)^3S_1$ level is selected as the initial level by the program). The designation INITIAL LEVEL used in the program printout refers to the lower state involved in the transition. The printout for a given initial level consists of the initial level identification with appropriate parameters, followed by a list of the allowed final levels. This list of final levels consists of (1) the final level identification and (2) the calculated transition parameters for that line (provided it is an emission line, i.e., $\lambda > 0$). Further, the final levels in the list are grouped as quadrupole transition levels (with subgroups $|\Delta L| = 0, 1, 2$) or dipole transition levels.

The output variables are presented with the printout variable name listed first and the program variable name (used internally in the program) listed next to it in brackets. The definition of the variable is given except when the variable has already been defined as an input variable.

A [AAAPN] dipole or quadrupole transition probability

ABS. OSCILLATOR STRENGTH [FAAPN] dipole absorption oscillator strength or f-value

CAPITAL L [CAPL(I)]

CAPITAL S [CAPS(I)]

DIFFERENCE [DIFF] $n_{l<} - n_{l>}$

ELEMENT NUMBER [ELEMNO]

J [J(N,I)] Nth J-value of the Ith term

LAMDA [XLAM] dipole or quadrupole transition wavelength in angstroms

LITTLE L [LLITT(I)]

LITTLE N [NLITT(I)]

N STAR OF LARGER LITTLE L VALUE [STARN(LGR)] $n_{l>}$ (where n is effective principal quantum number)

N STAR OF SMALLER LITTLE L VALUE [STARN(LSM)] $n_{l<}$

PARENT TERM CAPITAL L [CAPLP(I)]

PARENT TERM CAPITAL S [CAPSP(I)]

PARITY [PARITY(I)]

RAA [RAA(I)] $\langle r^2 \rangle$ for a given level

S [S] $\frac{S(\alpha, \alpha')}{a_0^4 e^2}$ quadrupole

S [SAAPN] $\frac{S(\alpha, \alpha')}{a_0^2 e^2}$ dipole

WAADP [WAADP] quadrupole transition angular frequency ($\omega = 2\pi f$ where f is frequency)

WAAP [WAAP] dipole transition angular frequency ($\omega = 2\pi f$ where f is frequency)

Z [Z]

This computer program was run on a Control Data 6600 computer system in which 14-place precision is standard. It is recommended that more than 8-place precision be employed if possible, since 8-place precision will give accurate Coulomb approximation results only for transitions with $n + n'$ less than approximately 10 (ref. 6).

Numerous comment cards have been incorporated into the listing of the computer program given in appendix A to assist the reader in understanding the functioning of the program.

The sample input deck in appendix A can be used as a test deck by comparing the printout generated for the initial level $2s(2S)^3S_1$ with the sample printout also given in appendix A.

RESULTS AND DISCUSSION

The results of calculating f-values for several transitions in neutral helium by several different methods are presented in table I. The f-values are averaged over the J-values of the initial levels by using the appropriate statistical weights and summed over the J-values of the final levels.

TABLE I.- ABSORPTION OSCILLATOR STRENGTHS FOR NEUTRAL HELIUM

Transition	Wiese, Smith, Glennon (ref. 13)	Coulomb approximation (a)	Self-consistent-field method	Scaled Thomas-Fermi method	Variational calculation of Goldberg (ref. 17)	Variational calculation of Hylleraas (ref. 18)	Sum rule modified calculation (ref. 19)	Coulomb approximation (b)	Effective charge method
1 ¹ S - 2 ¹ P	0.2762 SP	{ 0.2531 .06825 .02795 .01414 .008134 }	0.2719			0.3555			
3 ¹ P	.0734 SP		.07203			.0722			
4 ¹ P	.0302 W		.02738			.0282			
5 ¹ P	.0153 LS								
6 ¹ P	.00848 LS		.00793			.0082			
2 ¹ S - 2 ¹ P	.3764 SP	.3723	.3578	[.342]	0.389	.392	0.370	0.3719	0.3861
3 ¹ P	.1514 SP	.1492	.1646	.242	.157	.150	.156	.1431	.2948
4 ¹ P	.0507 W	.04865	.0508	.0684	.057	.062	.0503	.04970	.08728
5 ¹ P	.0221 DK	.02218		.0296	.0252	.025	.0221	.01936	.03818
6 ¹ P	.0128 T	.01209	.01257	.0157	.0136	.012	.0124		
2 ¹ P - 3 ¹ S	.0480 W	.04806	.04640	[.0278]		.04797		.04859	.02304
4 ¹ S	.00824 T	.008579	.00824	.00549		.00686		.008308	.004150
5 ¹ S	.00308 CA	.003213		.00211				.003041	.001519
6 ¹ S	.00153 T	.001593	.00151	.00105				.001491	.0007502
2 ¹ P - 3 ¹ D	.711 W	.7104	.7253	[.575]	.755	.7357		.7006	.6947
4 ¹ D	.122 T	.1207	.1205	.114	.118	.132		.1168	.1199
5 ¹ D	.0436 T	.04346	.04308	.0436	.0416	.04313		.04106	.04355
6 ¹ D	.0213 CA	.02105		.0218	.0199			.02054	.02115
2 ³ S - 2 ³ P	.5391 SP	.5457	.6002	.538	.542	.559	.535	.5319	.6686
3 ³ P	.06446 SP	.05982	.05705	.0638	.0826	.052	.0768	.06478	.1876
4 ³ P	.0231 W	.02370	.02083	.0256	.0270	.031	.0232	.02581	.06502
5 ³ P	.0114 DK	.01143		.0124	.0123	.013	.0114	.01022	.02999
6 ³ P	.00608 DK	.006372		.00694	.00665	.007	.0061		
2 ³ P - 3 ³ S	.0693 W	.06813	.07639	.0692		.07662		.07204	.02700
4 ³ S	.0118 T	.01014	.01159	.0105		.00520		.008939	.004288
5 ³ S	.00365 CA	.003581		.00376				.003159	.001488
6 ³ S	.00176 CA	.001720		.00182				.001527	.0007089
2 ³ P - 3 ³ D	.609 W	.6168	.6234	.611	.553	.6530		.6089	.6969
4 ³ D	.125 T	.1244	.1229	.123	.129	.0792		.1192	.1325
5 ³ D	.0474 T	.04759	.04668	.0472	.0512	.04951		.0455	.04958
6 ³ D	.0215 CA	.02374		.0236	.0260				.02446

^aCalculated by computer program in appendix A.^bCalculated by linear interpolation in original tables of Bates and Damgaard (ref. 5).

Notation:

- SP Results of variational calculations from reference 14.
W Results of variational calculations of A. W. Weiss presented in reference 13.
LS Results of Low and Stewart quoted in reference 15.
CA Coulomb approximation results presented in reference 13.
DK Results of reference 19 modified by Wiese, Smith, and Glennon (ref. 13).
T Results of reference 16 modified by Wiese, Smith, and Glennon (ref. 13).
[] Stewart-Rotenberg scaling factor is less than zero (see appendix D).
{ } Coefficient of fractional parentage used.

Perhaps the two most extensive sources of information on experimental and calculated f-values available to date are two National Bureau of Standards publications: namely, an extensive bibliography on atomic transition probabilities by Glennon and Wiese (ref. 12) and tables of atomic transition probabilities for hydrogen through neon selected after extensive evaluation of all available material by Wiese, Smith, and Glennon (ref. 13). The f-values chosen in reference 13 as the best values available are presented in the second column of table I. The results in this column include (1) those of A. W. Weiss calculated by a variational method in a manner similar to that used by Schiff and Pekeris (ref. 14), (2) Coulomb approximation results calculated by Wiese, Smith, and Glennon with a computer program made available to them by H. R. Griem, and (3) those of Low and Stewart (unpublished but quoted by Dalgarno and Stewart in ref. 15). Coulomb approximation results calculated by the computer program listed in appendix A, which uses the Coulomb approximation relations given in the present paper, are presented in the third column of table I. The self-consistent-field results including exchange effects (Hartree-Fock method) are those of Treffitz and associates (ref. 16). In addition to exchange effects, they attempt to take into account certain correlation effects, noncentral nature of the real system, and configuration mixing through the introduction of parameters of inter-electron distance. The scaled Thomas-Fermi results were made available by John Cooper of the Joint Institute for Laboratory Astrophysics, Boulder, Colorado. These results were calculated by the scaled Thomas-Fermi method of Stewart and Rotenberg (ref. 4). (See appendix D for discussion.) Also presented are the f-values obtained by the variational calculations of Goldberg (ref. 17) and Hylleraas (ref. 18) and f-values modified by Dalgarno and Kingston (ref. 19) such that they satisfy four different sum rules. Coulomb approximation results calculated by linear interpolation in the original Coulomb approximation tables of Bates and Damgaard (ref. 5) are listed in the ninth column of table I. Finally, results obtained by an effective charge method are given. The effective charge method utilizes eigenfunctions of the Schrödinger equation for hydrogen with an effective charge Z^* , where Z^* is chosen such that the hydrogenic energy eigenvalue equals the measured energy value $E_{n^*,l}$ of the system, that is,

$$Z^{*2} = \frac{n^{*2} E_{n^*,l}}{R_{\infty}} \quad (12)$$

where n^* is the integer principal quantum number.

A problem encountered in attempting to compare f-values calculated by several methods is the lack of knowledge of the true f-value and the difficulty in estimating the error introduced by the different approximations. In making comparisons among the present tabulated values, the values presented in reference 13 may be used as a general standard, although in certain cases, which are discussed, some of the present values may be more accurate.

For singlet transitions, the scaled Thomas-Fermi method is not rigorously applicable. The comparison of the new Coulomb approximation results (third column of table I) with the values from reference 13 is quite favorable. The good agreement of the Coulomb approximation f-values for triplet transitions with the values from reference 13 is immediately apparent. For triplet states, the scaled Thomas-Fermi method is applicable, and when significant differences exist between the scaled Thomas-Fermi results and the Coulomb approximation results, one can expect that these differences are due to significant contributions to the transition integral by the core region of the wave functions involved. As the levels involved in the transition become more highly excited levels, one expects the difference between the scaled Thomas-Fermi and Coulomb approximation results to decrease due to the decreasing contribution of the core regions for such wave functions. The results for the $2^3P - n^3D$ series in table I clearly show this trend with the $2^3P - 6^3D$ transition having the smallest difference for the series (about 0.6 percent compared with a 1.1 percent maximum for the series). However, this trend is not evident for the $2^3S - n^3P$ and $2^3P - n^3S$ series where the orbits involved are generally closer to the core. The average difference for the $2^3S - n^3P$ series (about 5.9 percent) is larger than that of the $2^3P - n^3S$ series (about 3.9 percent) as was to be expected due to the presence of the 2^3S level with large core penetration in each transition integral of the former series. For triplet transitions with a significant difference between the results of the two methods, the scaled Thomas-Fermi results can be expected to be the more accurate. The fact that some of these Coulomb approximation results are in better agreement with the values from reference 13 may not be significant.

The effective charge results are generally poor. This failure of the effective charge method can be attributed to the fact that the method fits a hydrogenic wave function for all values of r , including the generally insignificant core region. Although the Bates-Damgaard Coulomb approximation is poor in the core region, it is certainly best for larger values of r .

Reference 13 gives Coulomb approximation results as the best available values for several of the transitions listed in table I. For these cases, the present Coulomb approximation results (presented in the third column of table I) should be more accurate since the values from reference 13 were obtained by interpolation in the tables of Bates and Damgaard. Some feeling for the size of the errors introduced by such interpolation can be gained by comparing the present Coulomb approximation results in the third column of table I with the results in the ninth column of the table which were calculated by a computer program that interpolated linearly in the Bates-Damgaard tables. The results often differ in the second significant figure.

It was to be expected that the Coulomb approximation results for the series of transitions involving the ground state of neutral helium would, in general, be least accurate

due to the large contributions to the transition integral from the core region of the (two equivalent electron) ground state. The values from reference 13 for this series were all calculated from variational wave functions (one partial exception to this statement is the results of Low and Stewart ($1^1S - 5^1P$, $1^1S - 6^1P$; see ref. 15) who used modified hydrogenic wave functions for the upper levels and a variationally determined wave function for the ground state). The Coulomb approximation results for the $1^1S - n^1P$ series were obtained by multiplying the computer program results by the proper coefficients of fractional parentage, since the computer program does not handle equivalent electron transitions in its present form. The differences between the Coulomb approximation results and the values from reference 13 are indeed generally larger for this series of transitions than for any of the other series presented. The results for the $1^1S - 2^1P$ transition differ by about 8.7 percent, whereas those for the higher transitions in the series differ by not more than about 7.9 percent (the percent differences quoted are relative to average value of the two results). The self-consistent-field results are in better agreement with the values from reference 13 for the two lowest members of the series. For the other members of the series, the Coulomb approximation results are in better agreement than are the more sophisticated self-consistent-field results.

CONCLUDING REMARKS

The agreement of the Coulomb approximation f-values (absorption oscillator strengths) with the presently accepted f-values for neutral helium (i.e., the values from U.S. Dep. Com. NSRDS-NBS 4) is indeed satisfactory except for those transitions which involve the ground state. For most situations, where inaccuracies of about 10 percent in f-values can be tolerated, the Coulomb approximation f-values for the $1^1S - n^1P$ series are also adequate. While it should be understood that the Coulomb approximation may not work as well for other atoms, its nearly uniform success for neutral helium is impressive. The present results suggest that in situations where systematic calculations of large numbers of f-values or related quantities are required, the Coulomb approximation method should be used whenever applicable and be checked against the scaled Thomas-Fermi method when significant core contributions to the transition integral are expected. This procedure should reduce computing times considerably. The only alternative method for systematic calculations presently available is the self-consistent-field method which usually entails long computing times and which probably does not result in significant improvements over the scaled Thomas-Fermi method when the latter method is applicable (i.e., for those transitions which result in positive values for the Stewart and Rotenberg scaling factor). The variational method does not provide a

practical alternative for systematic calculations, since it involves time-consuming trial and error calculations and becomes exceedingly complex for excited states.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., July 31, 1970.

FORTRAN IV PROGRAM FOR CALCULATING DIPOLE AND
QUADRUPOLE TRANSITION PROBABILITIES

Computer Program Listing

18

APPENDIX A

```

125 FORMAT (1X11HDIFFERENCE=,F8.3)
126 FORMAT (1X3HA= ,E12.4//)
140 FORMAT(3I10,F10.1)
511 FORMAT(13H NOSER GT 10)
717 FORMAT(26H ABS. OSCILLATOR STRENGTH=E12.4,3H A=E12.4//)
833 FORMAT(//24H ERROR, WRONG TERM LIMIT)
834 FORMAT(/////3HEL=I3,4HLEV=I3,3H N=F5.1,3HSL=F5.1,3H S=F5.1,3HBL=F5
1.1,3H J=F5.1)
835 FORMAT(/////4H TJ=F12.2,10X6H TLIM=F12.2)
916 FORMAT(/////5H*****//)

```

```

C
C
C   DATA READ IN AND ORGANIZED
C
C
      READ(5,140) OPQUA,OPFVA,NPROP,NLITO
      READ(5,3) ELEMNO,Z,NOLEV,NOSER
100  DO 67 I=1,90
      TLIM(I)=0.
      IF(I.LT.11) SLIM(I)=0.
      67 CONTINUE
      I=0
      IF(NOSER.LE.10) GO TO 510
      PRINT 511
      STOP
510  CONTINUE
      I=I+1
      READ (5,7) (CAPSS(I),CAPLS(I),SLIM(I),I=1,NOSER)
      DO 10 I=1,NOLEV
      READ(5,6) NLITT(I),LLITT(I),CAPS(I),CAPL(I),PARITY(I),CAPSP(I),CAP
1LP(I)
      DO 9 M=1,NOSER
      IF(ABS(CAPSP(I)-CAPSS(M)).LT..5.AND.ABS(CAPLP(I)-CAPLS(M)).LT..5)
1 TLIM(I)=SLIM(M)
      9 CONTINUE

```

```

C
C   THE NUMBER OF J VALUES OF A TERM CALCULATED
C
      DIFF=ABS(CAPL(I)-CAPS(I))
      SUM=CAPL(I)+CAPS(I)
      NOJS(I)=SUM-DIFF+1.
      NOJ=NOJS(I)+.001

```

```

C
C   J ARRAY MUST BE IN ASCENDING ORDER
C
      READ(5,4) (TJ(N,I),N=1,NOJ)
      DO 801 N=1,NOJ
      XN=N
801  J(N,I)=DIFF+XN-.99999999

```

```

C
C   LOOPS 871,872 GENERATE MISSING TJ VALUES
C
      SAVET=0.
      DO 871 NK=1,NOJ
      IF(TJ(NK,I).LT.TLIM(I)) GO TO 871
      PRINT 833
      PRINT 834, NK,I,NLITT(I),LLITT(I),CAPSS(I),CAPLS(I),J(NK,I)
      PRINT 835, TJ(NK,I),TLIM(I)

```

APPENDIX A

```

871 CONTINUE
    DO 872 NK=1,NOJ
        IF(TJ(NK,I).LT.1.)TJ(NK,I)=SAVET
872 CONTINUE
10 CONTINUE

C
C
C    INITIAL LEVEL SELECTED AND ITS PARAMETERS CALCULATED
C
C
    DO 12 I=1,NOLEV
        X=0.0
        Y=0.0
        NOJ=NOJS(I)

C
C    CALCULATION OF AVERAGE TERM VALUE
C    (THE AVERAGE TERM VALUE IS THE AVERAGE OF THE ENERGY LEVEL VALUES,
C    EACH WEIGHTED BY THE APPROPRIATE STASTICAL WEIGHT, COMPOSING THE
C    TERM. THIS AVERAGE TERM VALUE IS USED TO CALCULATE THE EFFECTIVE
C    PRINCIPAL QUANTUM NUMBER FOR THE TERM. )
C
        DO 600 N=1,NOJ
            X=X+TJ(N,I)*(2.*J(N,I)+1.)
            Y=Y+2.*J(N,I)+1.
600 CONTINUE
        AVETJ(I)=X/Y

C
C    EFFECTIVE PRINCIPAL QUANTUM NUMBER CALCULATED FOR EACH TERM
C    ( SEE EQUATION (7) )
C
        STARN(I)=SQRT(Z**2*RYDBGD/(TLIM(I)-AVETJ(I)))
        CALL BATES(STARN(I),LLITT(I),STARN(I),LLITT(I),2.,Z,RAAI)
        RAA(I) = SQRT(RAAI)
12 CONTINUE

C
C    INITIAL LEVEL SELECTED
C
    DO 915 I=1,NOLEV
        NOJ=NOJS(I)
        DO 15 N=1,NOJ
            IF(NLITT(I).GT.9.5) GO TO 15

C
C    INITIAL LEVEL PRINTED OUT
C
        PRINT 118, ELEMNO,Z
        PRINT 109
        PRINT 102, NLITT(I),LLITT(I),CAPS(I),CAPL(I),PARITY(I)
        PRINT 111, CAPSP(I),CAPLP(I)
        PRINT 103, J(N,I),RAA(I)

C
C
C    DELTA CAPITAL L = 0 QUADRUPOLE TERMS
C
        IF(OPQUA.EQ.1) GO TO 760
        PRINT 101
        F=2.

```

APPENDIX A

```

DO 17 MN=1,NOLEV
C
C QUADRUPOLE SELECTION RULES APPLIED IN NEXT 8 STATEMENTS
C
IF(ABS(PARITY(I)-PARITY(MN)).GT..5)GO TO 17
IF(ABS(CAPS(I)-CAPS(MN)).GT..5) GO TO 17
IF(ABS(CAPL(I)-CAPL(MN)).GT..5) GO TO 17
IF(ABS(LLITT(I)+LLITT(MN)).LT..5) GO TO 17
IF(ABS(CAPSP(I)-CAPSP(MN)).GT..5) GO TO 17
IF(ABS(CAPLP(I)-CAPLP(MN)).GT..5) GO TO 17
IF(ABS(LLITT(I)-LLITT(MN)).GT.2.5) GO TO 17
IF(0.5.LT.ABS(LLITT(I)-LLITT(MN)).AND.ABS(LLITT(I)-LLITT(MN)).LT.1
1.5) GO TO 17
IF(ABS(NLITT(I)-NLITT(MN)).GT.NLITO) GO TO 17
C
C FINAL QUADRUPOLE LEVEL IDENTIFICATION PRINTED OUT
C
PRINT 110
PRINT 102, NLITT(MN),LLITT(MN),CAPS(MN),CAPL(MN),PARITY(MN)
PRINT 111, CAPSP(MN),CAPLP(MN)
C
C DISTINCTION MADE BETWEEN LEVELS WITH SMALLER AND LARGER LLITT
C
754 BIGSML=LLITT(I)
IF(LLITT(I)-LLITT(MN).LT.0.) BIGSML=LLITT(MN)
IF(ABS(BIGSML-LLITT(I)) .LT..5) LGR= I
IF(ABS(BIGSML-LLITT(MN)) .LT..5) LGR= MN
IF(ABS(BIGSML-LLITT(I)) .LT..5) LSM=MN
IF(ABS(BIGSML-LLITT(MN)) .LT..5) LSM=I
DIFF=STARN(LSM)-STARN(LGR)
IF(NPROP.NE.1) GO TO 905
C
C COULOMB APPROXIMATION QUADRUPOLE RADIAL MATRIX ELEMENT TABLE
C ENTRY POINTS PRINTED OUT
C
PRINT 113, STARN(LGR)
PRINT 114, STARN(LSM)
PRINT 125, DIFF
C
C SQUARE OF QUADRUPOLE RADIAL TRANSITION INTEGRAL CALAULATED
C
905 CALL BATES(STARN(I),LLITT(I),STARN(MN),LLITT(MN),F,Z,RSQAVE)
PRINT 104
CALL RACAH (LLITT(I),CAPL(I),LLITT(MN),CAPL(I),CAPLP(I),F,W2)
C
C PROPER COEFFICIENT CHOSEN FOR TRANSITIONS WITH EITHER 0 CHANGE,
C OR, + OR - 2 CHANGE IN LLITT. ( SEE EQUATION (C5) )
C
COEFF=2./3.*(2.*J(N,I)+1.)*(2.*CAPL(I)+1.)**2*RSQAVE
IF(ABS(LLITT(MN)-LLITT(I)).LT..5)COEFF=COEFF*BIGSML*(BIGSML+1.)*(2
1.*BIGSML+1.)/((2.*BIGSML-1.)*(2.*BIGSML+3.))
IF(ABS(ABS(LLITT(MN)-LLITT(I))-2.).LT..5)COEFF=COEFF*3.*(BIGSML-1.
1)*BIGSML/(2.*(2.*BIGSML-1.))
NO=NOJS(MN)
DO 16 M=1,NO
IF((TJ(M,MN)-TJ(N,I)).LT.0.)PRINT 107,J(M,MN)
IF((TJ(M,MN)-TJ(N,I)).LT.0.)GO TO 16
C

```

APPENDIX A

```

C      FURTHER QUADRUPOLE SELECTION RULES APPLIED IN THE NEXT 5 STATEMENTS
C
      IF(ABS(J(N,I)-J(M,MN)).GT.2.5) GO TO 16
      IF(ABS(J(N,I)+J(M,MN)).LT.1.2) GO TO 16
      IF(ABS(NLITT(I)-NLITT(MN)).GT..5) GO TO 751
      IF(ABS(LLITT(I)-LLITT(MN)).GT..5) GO TO 751
      IF(ABS(J(N,I)-J(M,MN)).LT..4) GO TO 17
751 CALL RACAH (CAPL(I),J(N,I),CAPL(I),J(M,MN),CAPS(I),F,W1)
C
C      QUADRUPOLE TRANSITION PARAMETERS CALCULATED AND PRINTED OUT
C
      S=COEFF*W1**2*W2**2*(2.*J(M,MN)+1.)
      IF(TJ(N,I).EQ.TJ(M,MN)) PRINT 115
      IF(TJ(N,I).EQ.TJ(M,MN)) GO TO 222
      WAADP=2.*PI*C*(TJ(N,I)-TJ(M,MN))*(-1.)
      XLAM=1.0E8/(TJ(N,I)-TJ(M,MN))*(-1.)
      PRINT 105,J(M,MN),S,WAADP,XLAM
      IF(OPFVA.NE.3) GO TO 16
      AAAPN=ALPHA*(AOBOHR/C)**4/(320.*(2.*J(M,MN)+1.))*WAADP**5*S
      PRINT 126,AAAPN
      GO TO 16
222 PRINT 119,J(M,MN),S
16 CONTINUE
17 CONTINUE
C
C      DELTA CAPITAL L = 1 QUADRUPOLE TERMS
C
      PRINT 106
      DO 310 M=1,NOLEV
      IF(ABS(NLITT(I)-NLITT(M)).GT.NLITO) GO TO 310
C
C      QUADRUPOLE SELECTION RULES APPLIED IN NEXT 8 STATEMENTS
C
      IF(ABS(PARITY(I)-PARITY(M)).GT..5) GO TO 310
      IF(ABS(CAPS(I)-CAPS(M)).GT..5) GO TO 310
      IF(ABS(ABS(CAPL(I)-CAPL(M))-1.).GT..5) GO TO 310
      IF(ABS(LLITT(I)+LLITT(M)).LT..5) GO TO 310
      IF(ABS(CAPSP(I)-CAPSP(M)).GT..5) GO TO 310
      IF(ABS(CAPLP(I)-CAPLP(M)).GT..5) GO TO 310
      IF(ABS(LLITT(I)-LLITT(M)).GT.2.5) GO TO 310
      IF(0.5.LT.ABS(LLITT(I)-LLITT(M)).AND.ABS(LLITT(I)-LLITT(M)).LT.1.5
1) GO TO 310
C
C      FINAL QUADRUPOLE LEVEL IDENTIFICATION PRINTED OUT
C
      PRINT 110
      PRINT 102, NLITT(M),LLITT(M),CAPS(M),CAPL(M),PARITY(M)
      PRINT 111, CAPSP(M),CAPLP(M)
C
C      DISTINCTION MADE BETWEEN LEVELS WITH SMALLER AND LARGER LLITT
C
      BIGSML=LLITT(I)
      IF(LLITT(I)-LLITT(M).LT.0.) BIGSML=LLITT(M)
      IF(ABS(BIGSML-LLITT(I)) .LT..5) LGR= I
      IF(ABS(BIGSML-LLITT(M)) .LT..5) LGR= M

```


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```

IF(ABS(BIGSML-LLITT(I)) .LT..5) LSM=M
IF(ABS(BIGSML-LLITT(M)) .LT..5) LSM=I
DIFF=STARN(LSM)-STARN(LGR)
IF(NPROP.NE.1) GO TO 904

C
C COULOMB APPROXIMATION QUADRUPOLE RADIAL MATRIX ELEMENT TABLE
C ENTRY POINTS PRINTED OUT
C

PRINT 113, STARN(LGR)
PRINT 114, STARN(LSM)
PRINT 125, DIFF

C
C SQUARE OF QUADRUPOLE RADIAL TRANSITION INTEGRAL CALAULATED
C

904 CALL BATES(STARN(I),LLITT(I),STARN(M),LLITT(M),F,Z,RSQAVE)
PRINT 104
CALL RACAH (LLITT(I),CAPL(I),LLITT(M),CAPL(M),CAPLP(I),F,W3)

C
C PROPER COEFFICIENT CHOSEN FOR TRANSITIONS WITH EITHER 0 CHANGE,
C OR, + OR - 2 CHANGE IN LLITT. ( SEE EQUATION (C5) )
C

COEFF=2./3.*(2.*J(N,I)+1.)*(2.*CAPL(I)+1.)*(2.*CAPL(M)+1.)*W3**2*RSQAVE
IF(ABS(LLITT(M)-LLITT(I)).LT..5) COEFF=COEFF*BIGSML*(BIGSML+1.)*(2
1.*BIGSML+1.)/((2.*BIGSML-1.)*(2.*BIGSML+3.))
IF(ABS(ABS(LLITT(M)-LLITT(I))-2.).LT..5) COEFF=COEFF*3.*(BIGSML-1.)
1.*BIGSML/(2.*(2.*BIGSML-1.))
NO=NOJS(M)
DO 33 NX=1,NO
IF((TJ(NX,M)-TJ(N,I)).LT.0.)PRINT 107,J(NX,M)
IF((TJ(NX,M)-TJ(N,I)).LT.0.)GO TO 33

C
C FURTHER QUADRUPOLE SELECTION RULES APPLIED IN THE NEXT 5 STATEMENTS
C

IF(ABS(J(NX,M)-J(N,I)).GT.2.5) GO TO 33
IF(ABS(J(NX,M)+J(N,I)).LT.1.2) GO TO 33
IF(ABS(NLITT(I)-NLITT(M)).GT..5) GO TO 752
IF(ABS(LLITT(I)-LLITT(M)).GT..5) GO TO 752
IF(ABS(J(N,I)-J(NX,M)).LT..4) GO TO 310
752 CALL RACAH (CAPL(I),J(N,I),CAPL(M),J(NX,M),CAPS(I),F,W4)

C
C QUADRUPOLE TRANSITION PARAMETERS CALCULATED AND PRINTED OUT
C

S=COEFF*W4**2*(2.*J(NX,M)+1.)
IF(TJ(N,I).EQ.TJ(NX,M))PRINT 115
IF(TJ(N,I).EQ.TJ(NX,M))GO TO 333
WAADP=2.*PI*C*(TJ(N,I)-TJ(NX,M))*(-1.)
XLAM=1.0E8/(TJ(N,I)-TJ(NX,M))*(-1.)
PRINT 105,J(NX,M),S,WAADP,XLAM
IF(OPFVA.NE.3) GO TO 33
AAAPN=ALPHA*(AOBOHR/C)**4/(320.*(2.*J(NX,M)+1.))*WAADP**5*S
PRINT 126,AAAPN
GO TO 33
333 PRINT 119,J(NX,M),S
33 CONTINUE
310 CONTINUE
C

```

APPENDIX A

```

C
C DELTA CAPITAL L = 2 QUADRUPOLE TERMS
C
C PRINT 108
C DO 31 M=1,NOLEV
C IF(ABS(NLITT(I)-NLITT(M)).GT.NLITO) GO TO 31
C
C QUADRUPOLE SELECTION RULES APPLIED IN NEXT 8 STATEMENTS
C
C IF(ABS(PARITY(I)-PARITY(M)).GT..5) GO TO 31
C IF(ABS(CAPS(I)-CAPS(M)).GT..5) GO TO 31
C IF(ABS(ABS(CAPL(I)-CAPL(M))-2.).GT..5) GO TO 31
C IF(ABS(LLITT(I)+LLITT(M)).LT..5) GO TO 31
C IF(ABS(CAPSP(I)-CAPSP(M)) .GT..5) GO TO 31
C IF(ABS(CAPLP(I)-CAPLP(M)) .GT..5) GO TO 31
C IF(ABS(LLITT(I)-LLITT(M)).GT.2.5) GO TO 31
C IF(0.5.LT.ABS(LLITT(I)-LLITT(M)).AND.ABS(LLITT(I)-LLITT(M)).LT.1.5
1) GO TO 31
C
C FINAL QUADRUPOLE LEVEL IDENTIFICATION PRINTED OUT
C
C PRINT 110
C PRINT 102, NLITT(M),LLITT(M),CAPS(M),CAPL(M),PARITY(M)
C PRINT 111, CAPSP(M),CAPLP(M)
C
C DISTINCTION MADE BETWEEN LEVELS WITH SMALLER AND LARGER LLITT
C
C BIGSML=LLITT(I)
C IF(LLITT(I)-LLITT(M).LT.0.) BIGSML=LLITT(M)
C IF(ABS(BIGSML-LLITT(I)) .LT..5) LGR= I
C IF(ABS(BIGSML-LLITT(M)) .LT..5) LGR= M
C IF(ABS(BIGSML-LLITT(I)) .LT..5) LSM=M
C IF(ABS(BIGSML-LLITT(M)) .LT..5) LSM=M
C DIFF=STARN(LSM)-STARN(LGR)
C IF(NPROP.NE.1) GO TO 903
C
C COULOMB APPROXIMATION QUADRUPOLE RADIAL MATRIX ELEMENT TABLE
C ENTRY POINTS PRINTED OUT
C
C PRINT 113, STARN(LGR)
C PRINT 114, STARN(LSM)
C PRINT 125, DIFF
C
C SQUARE OF QUADRUPOLE RADIAL TRANSITION INTEGRAL CALAULATED
C
903 CALL BATES(STARN(I),LLITT(I),STARN(M),LLITT(M),F,Z,RSQAVE)
C PRINT 104
C CALL RACAH (LLITT(I),CAPL(I),LLITT(M),CAPL(M),CAPLP(I),F,W5)
C
C PROPER COEFFICIENT CHOSEN FOR TRANSITIONS WITH EITHER 0 CHANGE,
C OR, + OR - 2 CHANGE IN LLITT. ( SEE EQUATION (C5) )
C
C COEFF=2.*(2.*J(N,I)+1.)*(2.*CAPL(I)+1.)*(2.*CAPL(M)+1.)*W5**2*RSQA
C 1VE/3.
C IF(ABS(LLITT(M)-LLITT(I)).LT..5)COEFF=COEFF*BIGSML*(BIGSML+1.)*(2.
C 1 *BIGSML+1.)/((2.*BIGSML-1.)*(2.*BIGSML+3.))

```

APPENDIX A

```

      IF(ABS(ABS(LLITT(M)-LLITT(I))-2.) .LT..5) COEFF=COEFF*3.*(BIGSML-1.)
1  *BIGSML/(2.*(2.*BIGSML-1.))
      NO=NOJS(M)
      DO 699 NX=1,NO
      IF((TJ(NX,M)-TJ(N,I)).LT.0.) PRINT 107,J(NX,M)
      IF((TJ(NX,M)-TJ(N,I)).LT.0.) GO TO 699
C
C      FURTHER QUADRUPOLE SELECTION RULES APPLIED IN THE NEXT 5 STATEMENTS
C
      IF(ABS(J(NX,M)-J(N,I)) .GT.2.5) GO TO 699
      IF(ABS(J(NX,M)+J(N,I)).LT.1.2) GO TO 699
      IF(ABS(NLITT(I)-NLITT(M)) .GT..5) GO TO 753
      IF(ABS(LLITT(I)-LLITT(M)) .GT..5) GO TO 753
      IF(ABS(J(N,I)-J(NX,M)).LT..4) GO TO 31
753 CALL RACAH (CAPL(I),J(N,I),CAPL(M),J(NX,M),CAPS(I),F,W6)
C
C      QUADRUPOLE TRANSITION PARAMETERS CALCULATED AND PRINTED OUT
C
      S=COEFF*W6**2*(2.*J(NX,M)+1.)
      IF(TJ(N,I).EQ.TJ(NX,M)) PRINT 115
      IF(TJ(N,I).EQ.TJ(NX,M)) GO TO 444
      WAADP=2.*PI*C*(TJ(N,I)-TJ(NX,M))*(-1.)
      XLAM=1.0E8/(TJ(N,I)-TJ(NX,M))*(-1.)
      PRINT 105,J(NX,M),S,WAADP,XLAM
      IF(OPFVA.NE.3) GO TO 699
      AAAPN=ALPHA*(AOBOHR/C)**4/(320.*(2.*J(NX,M)+1.))*WAADP**5*S
      PRINT 126,AAAPN
      GO TO 699
444 PRINT 119,J(NX,M),S
699 CONTINUE
31 CONTINUE
C
C      DIPOLE TERMS
C
C
760 CONTINUE
      F=1.
      PRINT 112
      DO 50 M=1,NOLEV
      IF(ABS(NLITT(I)-NLITT(M)).GT.NLITO) GO TO 50
C
C      DIPOLE SELECTION RULES APPLIED IN THE NEXT 7 STATEMENTS
C
      IF(ABS(CAPLP(I)-CAPLP(M)) .GT..5) GO TO 50
      IF(ABS(CAPSP(I)-CAPSP(M)) .GT..5) GO TO 50
      IF(ABS(ABS(PARITY(I)-PARITY(M))-2.) .GT..5) GO TO 50
      IF(ABS(CAPL(I)-CAPL(M)) .GT.1.5) GO TO 50
      IF(ABS(CAPL(I)+CAPL(M)).LT.0.5) GO TO 50
      IF(ABS(CAPS(I)-CAPS(M)) .GT..5) GO TO 50
      IF(ABS(ABS(LLITT(I)-LLITT(M))-1.) .GT..5) GO TO 50
C
C      DISTINCTION MADE BETWEEN LEVELS WITH SMALLER AND LARGER LLITT
C
      BIGSML=LLITT(I)
      IF(LLITT(I)-LLITT(M).LT.0.) BIGSML=LLITT(M)
      IF(ABS(BIGSML-LLITT(I)) .LT..5) LGR= I

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IF(ABS(BIGSML-LLITT(M)) .LT..5) LGR= M
IF(ABS(BIGSML-LLITT(I)) .LT..5) LSM=M
IF(ABS(BIGSML-LLITT(M)) .LT..5) LSM=I
P=9.*STARN(LGR)**2*ABS(STARN(LGR)**2-BIGSML**2)/(Z**2*4.*(4.*BIGSM
1L**2-1.))
DIFF=STARN(LSM)-STARN(LGR)
C
C FINAL DIPOLE LEVEL IDENTIFICATION PRINTED OUT
C
PRINT 110
PRINT 102, NLITT(M), LLITT(M), CAPS(M), CAPL(M), PARITY(M)
PRINT 111, CAPSP(M), CAPLP(M)
IF(NPROP.NE.1) GO TO 707
C
C COULOMB APPROXIMATION DIPOLE RADIAL MATRIX ELEMENT TABLE ENTRY
C POINTS PRINTED OUT
C
PRINT 113, STARN(LGR)
PRINT 114, STARN(LSM)
PRINT 125, DIFF
707 STARNL=STARN(LGR)
C
C SQUARE OF DIPOLE RADIAL TRANSITION INTEGRAL CALCULATED
C
CALL BATES(STARN(I), LLITT(I), STARN(M), LLITT(M), F, Z, RSQAVE)
PHISQ=RSQAVE*4.*Z**2/(9.*STARNL**2*ABS(STARNL**2-BIGSML**2))
708 PRINT 116
CALL RACAH (LLITT(I), CAPL(I), LLITT(M), CAPL(M), CAPLP(I), F, W7)
NO=NOJS(M)
DO 49 NX=1, NO
IF((TJ(NX, M)-TJ(N, I)).LT.0.) PRINT 107, J(NX, M)
IF((TJ(NX, M)-TJ(N, I)).LT.0.) GO TO 49
C
C FURTHER DIPOLE SELECTION RULES APPLIED IN THE NEXT 2 STATEMENTS
C
IF(ABS(J(N, I)+J(NX, M)).LT.0.5) GO TO 49
IF(ABS(J(N, I)-J(NX, M)) .GT.1.5) GO TO 49
CALL RACAH (CAPL(I), J(N, I), CAPL(M), J(NX, M), CAPS(I), F, W8)
C
C DIPOLE TRANSITION PARAMETERS CALCULATED AND PRINTED OUT
C
46 SRAAP=(2.*J(NX, M)+1.)*(2.*CAPL(I)+1.)*(2.*CAPL(M)+1.)*BIGSML*(4.*B
1IGSML**2-1.)*W7**2*W8**2
PRAAP=SRAAP*P
RAAP=PHISQ*PRAAP
SAAPN=RAAP *(2.*J(N, I)+1.)
IF(TJ(N, I).EQ.TJ(NX, M)) PRINT 115
IF(TJ(N, I).EQ.TJ(NX, M)) GO TO 555
WAAP=2.*PI*C*(TJ(N, I)-TJ(NX, M))*(-1.)
XLAM=-1E9/(TJ(N, I)-TJ(NX, M))*(-1.)
700 PRINT 105, J(NX, M), SAAPN, WAAP, XLAM
IF(OPFVA.EQ.2) GO TO 49
FAAPN=2.*AOBOHR/(3.*ALPHA*C*(2.*J(N, I)+1.))*WAAP*SAAPN
AAAPN=4.*ALPHA*AOBOHR**2/(3.*C**2*(2.*J(NX, M)+1.))*WAAP**3*SAAPN
PRINT 717, FAAPN, AAAPN
GO TO 49
555 PRINT 119, J(NX, M), SAAPN

```

APPENDIX A

```

49 CONTINUE
50 CONTINUE
15 CONTINUE
915 CONTINUE
    PRINT 916
    STOP
    END

```

C
C
C
C
C

RACAH COEFFICIENTS CALCULATED (SEE EQUATION (10))

```

SUBROUTINE RACAH(A,B,C,D,E,F,W)
W=0.
CALL DELTA(A,B,E,D1)
CALL DELTA(B,D,F,D2)
CALL DELTA(A,F,C,D3)
CALL DELTA(E,D,C,D4)
SUM=0.0
DO 10 N=1,20
X=N
Y=X+.000001
T1=Y-A-B-E
T2=Y-B-D-F
T3=Y-A-F-C
T4=Y-E-D-C
T5=A+B+C+D-X
T6=A+D+E+F-X
T7=B+C+E+F-X
IF(T1.LT.-.5)GO TO 10
IF(T2.LT.-.5)GO TO 10
IF(T3.LT.-.5)GO TO 10
IF(T4.LT.-.5)GO TO 10
IF(T5.LT.-.5)GO TO 11
IF(T6.LT.-.5)GO TO 11
IF(T7.LT.-.5)GO TO 11
DENOM= GAMMF(T1+1.,0)* GAMMF(T2+1.,0)* GAMMF(T3+1.,0)*
1 GAMMF(T4+1.,0)* GAMMF(T5+1.,0)* GAMMF(T6+1.,0)*GAMMF(T7+1.,0)
XNUM= (-1.)*N*GAMMF(X+2.,0)
SUM=SUM+XNUM/DENOM
10 CONTINUE
11 K=A+B+C+D
W=(-1.)*K*D1*D2*D3*D4*SUM
RETURN
END

```

C
C
C
C
C

THE DELTA FUNCTION CALCULATED (SEE EQUATION (11))

```

SUBROUTINE DELTA(EM,EN,EL,D)
D=0.
IF(EM+EL-EN.LT.-.5)GO TO 20
IF(EN+EL-EM.LT.-.5)GO TO 20
IF(EM+EN-EL.LT.-.5)GO TO 20
GT= GAMMF(EM+EN-EL+1.,0)*GAMMF(EN+EL-EM+1.,0)* GAMMF(EL+EM-EN+1.
1 ,0)/GAMMF(EM+EN+EL+2.,0)

```

APPENDIX A

```

      IF(GT.LT.0.) WRITE(6,10) EM,EN,EL
10  FORMAT(18H IN DELTA GT NEG,3E17.8)
      D= SQRT(GT)
20  CONTINUE
      RETURN
      END

```

C
C
C
C
C
C

SQUARE OF THE COULOMB APPROXIMATION RADIAL TRANSITION INTEGRAL
CALCULATED (SEE EQUATIONS (6),(8),(9))

```

SUBROUTINE BATES(STAR,L,STARP,LP,ALFA,Z,RSQUAR)
DIMENSION A(50),AP(50)
REAL L,LP
IF(STAR-L.LT..2) GO TO 15
IF(STARP-LP.LT..2) GO TO 15
MAX=STAR+STARP+ALFA-.99
S=STAR+STARP
A(1)=1.
AP(1)=1.
IF(MAX.LT.2) GO TO 11
DO 10 I=2,MAX
XI=I-1
A(I)=A(I-1)*(-1.)*STAR*(STAR-L-XI)*(STAR+L-XI+1.)/(2.*XI)
AP(I)=AP(I-1)*(-1.)*STARP*(STARP-LP-XI)*(STARP+LP-XI+1.)/(2.*XI)
10 CONTINUE
30 GT= GAMMF(STAR+L+1.,0)*GAMMF(STAR-L,0)*GAMMF(STARP+LP+1.,0)
1 *GAMMF(STARP-LP,0)
IF(GT.LT.0.) WRITE(6,20) STAR,L,STARP
20 FORMAT(  H IN BATES GT NEG,3E17.8)
11 F=2.**S*STAR**(STARP+ALFA+2.)*STARP**(STAR+ALFA+2.)/(S**(S+ALFA+3.
1)*Z**ALFA* SQRT(GT))
MAX=MAX+1
14 SUM=0.
DO 12 K=1,MAX
DO 13 KP=1,MAX
IF(K+KP.GT.MAX) GO TO 12
IF(STAR+STARP+3.+ALFA-FLOAT(K+KP).LT..2) GO TO 15
SUM=SUM+A(K)*AP(KP)*(1./STAR+1./STARP)**(K+KP)*GAMMF(S*ALFA+3.-FLO
1AT(K+KP),0)
13 CONTINUE
12 CONTINUE
SUM=SUM*F
RSQUAR=SUM**2
GO TO 16
15 RSQUAR=0.
16 RETURN
      END

```

APPENDIX A

Sample Input Deck

```

C   CARD 1 ( OPTIONS )
C   OPQUA,OPFVA,NPROP,NLITO
      2      3      1      2.0

C   CARD 2 ( ATOMIC SYSTEM DEFINED, HELIUM I )
C   ELEMNO,Z,NOLEV,NOSER
      2   1.   6   1

C   CARD 3 ( THERE IS ONLY 1 CARD LIKE CARD 3, SINCE HE I HAS ONLY 1 SERIES )
C   CAPSS(I),CAPLS(I),SLIM(I)
      .5   0.  198305.7

C   THE REMAINING DATA CARDS ARE IN TWO-CARD SEQUENCES WITH ONE TWO-CARD
C   SEQUENCE FOR EACH INPUT LEVEL ( THUS THERE ARE SIX TWO-CARD SEQUENCES,
C   SINCE NOLEV = 6 )

C   1ST CARD OF 1ST SEQUENCE
C   NLITT(1),LLITT(1),CAPS(1),CAPL(1),PARITY(1),CAPSP(1),CAPLP(1)
      2.   0.   1.   0.   2.   0.5  0.

C   2ND CARD OF 1ST SEQUENCE
C   TJ(N,1),N=1,NOJ (1ST LEVEL )
      159850.318

C   1ST CARD OF 2ND SEQUENCE
C   NLITT(2),LLITT(2),CAPS(2),CAPL(2),PARITY(2),CAPSP(2),CAPLP(2)
      2.   1.   1.   1.   0.   0.5  0.

C   2ND CARD OF 2ND SEQUENCE
C   TJ(N,2),N=1,NOJ (2ND LEVEL )
      169082.185  169081.189  169081.111

```

APPENDIX A

C 1ST CARD OF 3RD SEQUENCE
C NLITT(3),LLITT(3),CAPS(3),CAPL(3),PARITY(3),CAPSP(3),CAPLP(3)

3. 1. 1. 1. 0. 0.5 0.

C 2ND CARD OF 3RD SEQUENCE
C TJ(N,3),N=1,NOJ (3RD LEVEL)

185559.277 185559.085 185558.920

C 1ST CARD OF 4TH SEQUENCE
C NLITT(4),LLITT(4),CAPS(4),CAPL(4),PARITY(4),CAPSP(4),CAPLP(4)

3. 2. 1. 2. 2. 0.5 0.

C 2ND CARD OF 4TH SEQUENCE
C TJ(N,4),N=1,NOJ (4TH LEVEL)

186095.900 186095.900 186095.900

C 1ST CARD OF 5TH SEQUENCE
C NLITT(5),LLITT(5),CAPS(5),CAPL(5),PARITY(5),CAPSP(5),CAPLP(5)

4. 1. 1. 1. 0. 0.5 0.

C 2ND CARD OF 5TH SEQUENCE
C TJ(N,5),N=1,NOJ (5TH LEVEL)

191211.420 191211.420 191211.400

C 1ST CARD OF 6TH SEQUENCE
C NLITT(6),LLITT(6),CAPS(6),CAPL(6),PARITY(6),CAPSP(6),CAPLP(6)

4. 2. 1. 2. 2. 0.5 0.

C 2ND CARD OF 6TH SEQUENCE
C TJ(N,6),N=1,NOJ (6TH LEVEL)

191438.830 191438.830 191438.830

APPENDIX A

Sample Printout

C
C HELIUM 1
C OPTION VARIABLE VALUES ARE OPQUA=2,OPFVA=3,NPROP=1,NLITO=2.0
C

ELEMENT NUMBER, 2, WITH Z= 1
INITIAL LEVEL
LITTLE N= 2, LITTLE L= 0, CAPITAL S= 1.0, CAPITAL L= 0.0, PARITY= 2
PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0
INITIAL J VALUE J= 1.0, RAA= 21.790

DELTA L EQUALS 0 QUADRUPOLE TERMS

DELTA L EQUALS 1 QUADRUPOLE TERMS

DELTA L EQUALS 2 QUADRUPOLE TERMS

FINAL LEVEL
LITTLE N= 3, LITTLE L= 2, CAPITAL S= 1.0, CAPITAL L= 2.0, PARITY= 2
PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0
N STAR OF LARGER LITTLE L VALUE= 2.998
N STAR OF SMALLER LITTLE L VALUE= 1.689
DIFFERENCE= -1.309

FINAL J VALUES	S	WAADP	LAMDA
1.0	2.6306E+02	4.9438E+15	3810.2
A= 5.7319E+00			

2.0	4.3842E+02	4.9438E+15	3810.2
A= 5.7319E+00			

3.0	6.1379E+02	4.9438E+15	3810.2
A= 5.7319E+00			

FINAL LEVEL
LITTLE N= 4, LITTLE L= 2, CAPITAL S= 1.0, CAPITAL L= 2.0, PARITY= 2
PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0
N STAR OF LARGER LITTLE L VALUE= 3.998
N STAR OF SMALLER LITTLE L VALUE= 1.689
DIFFERENCE= -2.308

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FINAL J VALUES	S	WAADP	LAMDA
1.0	3.4744E+01	5.9502E+15	3165.7
A= 1.9120E+00			
2.0	5.7907E+01	5.9502E+15	3165.7
A= 1.9120E+00			
3.0	8.1069E+01	5.9502E+15	3165.7
A= 1.9120E+00			

DIPOLE TERMS

FINAL LEVEL
 LITTLE N= 2, LITTLE L= 1, CAPITAL S= 1.0, CAPITAL L= 1.0, PARITY= 0
 PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0
 N STAR OF LARGER LITTLE L VALUE= 1.938
 N STAR OF SMALLER LITTLE L VALUE= 1.689
 DIFFERENCE= -.249
 FINAL J VALUES S WAAP LAMDA
 .0 6.4877E+00 1.7390E+15 10832.0
 ABS. OSCILLATOR STRENGTH= 6.0643E-02 A= 1.0342E+07

1.0 1.9463E+01 1.7390E+15 10832.0
 ABS. OSCILLATOR STRENGTH= 1.8191E-01 A= 1.0338E+07

2.0 3.2438E+01 1.7390E+15 10832.0
 ABS. OSCILLATOR STRENGTH= 3.0318E-01 A= 1.0338E+07

FINAL LEVEL
 LITTLE N= 3, LITTLE L= 1, CAPITAL S= 1.0, CAPITAL L= 1.0, PARITY= 0
 PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0
 N STAR OF LARGER LITTLE L VALUE= 2.934
 N STAR OF SMALLER LITTLE L VALUE= 1.689
 DIFFERENCE= -1.245
 FINAL J VALUES S WAAP LAMDA
 .0 2.5533E-01 4.8426E+15 3889.7
 ABS. OSCILLATOR STRENGTH= 6.6464E-03 A= 8.7900E+06

1.0 7.6598E-01 4.8426E+15 3889.7
 ABS. OSCILLATOR STRENGTH= 1.9939E-02 A= 8.7898E+06

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2.0 1.2766E+00 4.8426E+15 3889.7
 ABS. OSCILLATOR STRENGTH= 3.3231E-02 A= 8.7896E+06

FINAL LEVEL

LITTLE N= 4, LITTLE L= 1, CAPITAL S= 1.0, CAPITAL L= 1.0, PARITY= 0

PARENT TERM CAPITAL S= .5, CAPITAL L= 0.0

N STAR OF LARGER LITTLE L VALUE= 3.933

N STAR OF SMALLER LITTLE L VALUE= 1.689

DIFFERENCE= -2.244

FINAL J VALUES S WAAP LAMDA
 .0 8.2923E-02 5.9073E+15 3188.7

ABS. OSCILLATOR STRENGTH= 2.6331E-03 A= 5.1819E+06

1.0 2.4877E-01 5.9073E+15 3188.7
 ABS. OSCILLATOR STRENGTH= 7.8994E-03 A= 5.1819E+06

2.0 4.1461E-01 5.9073E+15 3188.7
 ABS. OSCILLATOR STRENGTH= 1.3166E-02 A= 5.1819E+06

APPENDIX B

RELATIVE LINE AND MULTIPLY STRENGTHS FOR DIPOLE TRANSITIONS

In the notation of Shore and Menzel (ref. 20), the line strength may be factored as

$$S(\alpha, \alpha') = S(\alpha', \alpha) = R_{\text{line}}^2 R_{\text{mult}}^2 I^2 \quad (\text{B1})$$

where R_{line} and R_{mult} are the line factor and multiplet factor, respectively, and I the radial factor. They are related to the customary relative line and multiplet strengths (tabulated by Goldberg in refs. 21 and 22) and the radial factor σ by

$$S(\text{line}) = \frac{R_{\text{line}}^2}{2S + 1} \quad (\text{B2})$$

$$S(\text{mult}) = l_{>}(2S + 1)(4l_{>}^2 - 1)R_{\text{mult}}^2 \quad (\text{B3})$$

$$\sigma^2 = \frac{I^2}{l_{>}(4l_{>}^2 - 1)} \quad (\text{B4})$$

where S is the total atomic spin quantum number and $l_{>}$ is the larger of the individual electron orbital angular momentum quantum numbers l and l' .

The radial factor I is related to the radial transition integral I_S by

$$I = (-1)^{l_{>}-l} \sqrt{l_{>}} I_S \quad (\text{B5})$$

Under the restrictions of LS coupling and transitions involving no equivalent electrons, the relative line and multiplet strengths can be expressed in terms of Racah coefficients $W(abcd;ef)$ (ref. 9) as

$$S(\text{line}) = \frac{(2J + 1)(2J' + 1)}{(2S + 1)} W^2(LJL'J';S1) \quad (\text{B6})$$

and

$$S(\text{mult}) = (2S + 1)(2L + 1)(2L' + 1)l_{>}(4l_{>}^2 - 1)W^2(lLl'L';L_11) \quad (\text{B7})$$

The usual notation has been used for the total atomic orbital angular momentum quantum number L and the total atomic angular momentum quantum number J ; the subscript 1 indicates that the quantum number refers to the parent configuration. Racah coefficients

APPENDIX B

can be found in tabular form (ref. 10) or can be calculated by computer (eq. (10)). In order to generalize the results to equivalent electron configurations, coefficients of fractional parentage are required (ref. 20).

APPENDIX C

QUADRUPOLE RELATIONS

For quadrupole transitions (ref. 23), the transition probability can be expressed in terms of the quadrupole line strength as

$$A(\alpha, \alpha') = \frac{1}{320} \left(\frac{e^2}{\hbar c} \right)^6 \frac{c}{a_0} \frac{1}{g_{\alpha'}} \left(\frac{|T_{\alpha} - T_{\alpha'}|}{R_{\infty}} \right)^5 \frac{S(\alpha, \alpha')}{e^2 a_0^4} \quad (C1)$$

The quadrupole line strength can be factored analogously to the dipole line strength as

$$S(\alpha, \alpha') = S(\alpha', \alpha) = \frac{2}{3} R_{\text{line}}^2 R_{\text{mult}}^2 I^2 \quad (C2)$$

where the angular factors can be expressed as

$$R_{\text{line}} = (-1)^{S-L-J'} \left[(2J+1)(2J'+1) \right]^{1/2} W(LJL'J'; S2) \quad (C3)$$

and

$$R_{\text{mult}} = (-1)^{L_1-L-L'} \left[(2L+1)(2L'+1) \right]^{1/2} W(LL'L'; L_1 2) \quad (C4)$$

The radial factor is given by

$$I = \begin{cases} \left[\frac{l(l+1)(2l+1)}{(2l-1)(2l+3)} \right]^{1/2} I_2 & (\Delta l = 0 \text{ transitions}) \\ - \left[\frac{3(l_{<}+1)(l_{<}+2)}{2(2l_{<}+3)} \right]^{1/2} I_2 & (\Delta l = \pm 2 \text{ transitions}) \end{cases} \quad (C5)$$

where I_2 is the quadrupole radial transition integral I_s (defined by eq. (6)) with $s = 2$.

APPENDIX D

SCALED THOMAS-FERMI METHOD

The scaled Thomas-Fermi method of Stewart and Rotenberg (ref. 4) makes use of the Thomas-Fermi statistical model of atoms and ions. The potential due to the core of a multiple electron atom can be approximated by the potential of an appropriate Thomas-Fermi ion at all radial distances (since outside the Thomas-Fermi ion the potential becomes the correct Coulombic one), namely a Thomas-Fermi ion with net charge and nuclear charge equal to the core charge and nuclear charge of the actual atom or ion, respectively. Stewart and Rotenberg introduce a scaling factor which allows for uniform contraction and dilatation of the Thomas-Fermi core in an effort to compensate for the inadequacies of the Thomas-Fermi model. The scaling factor is determined by requiring that the energy parameter be identical to the measured energy value of the system. Stewart and Rotenberg have shown that the wave functions obtained by the scaled Thomas-Fermi method compare favorably with the wave functions obtained by the more sophisticated self-consistent-field method. In the region outside the Thomas-Fermi core, the scaled Thomas-Fermi method yields radial wave functions which are identical to the Bates-Damgaard Coulomb approximation wave functions except for a difference in the normalization factor.

A problem sometimes encountered in applying the scaled Thomas-Fermi method deserves mention. A Thomas-Fermi ion exists only when the binding energy of the system is greater than the corresponding hydrogenic value. When this requirement is not met, a negative Stewart-Rotenberg scaling factor results which implies that the Thomas-Fermi ion has a radius smaller than zero, that is, no Thomas-Fermi ion exists. In such cases the Bates-Damgaard Coulomb approximation should be used.

Such a situation exists in neutral helium for all the singlet states given in table I. Instead of abandoning the scaled Thomas-Fermi method for the singlet states, the binding energies of the singlet states were replaced by the average energies obtained from

$$E_{av} = \frac{E(\text{singlet}) + 3E(\text{triplet})}{4} \quad (D1)$$

This artifact makes the Stewart-Rotenberg scaling factor positive and finite for all the singlet states. The results of these calculations for the singlet states are presented in table I (enclosed in brackets), but in general they may be expected to be less accurate than the corresponding Coulomb approximation results.

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